

Hormone Activity of Hydroxylated Polybrominated Diphenyl Ethers to Human Thyroid Receptors β : *in Vitro* and *in Silico* Investigations

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Table S1. Values and some statistics of selected molecular structural descriptors for the QSAR model development

Compounds ^a	logK _{OW}	<i>V</i> (cm ³ /mol)	α (a.u.) ^b	μ (debye)	<i>E</i> _{HOMO} (eV)	<i>E</i> _{LUMO} (eV)	<i>q</i> _{OH} (a.c.u.) ^c	<i>q</i> _{OH} (a.c.u.)	<i>q</i> _O (a.c.u.)	ω (eV)	<i>I</i> _A	<i>n</i> _{Br}
3'-OH-BDE-7*	4.84	185.07	193.56	1.93	-6.43	-1.27	0.25	-0.25	0.06	2.87	0.98	2
4'-OH-BDE-17	5.67	214.25	212.43	4.41	-6.56	-1.41	0.25	-0.25	0.05	3.08	0.97	3
3'-OH-BDE-28	5.67	190.19	218.12	1.40	-6.45	-1.43	0.26	-0.19	0.05	3.09	0.98	3
2'-OH-BDE-28	5.67	158.11	216.09	1.26	-6.62	-1.54	0.28	-0.24	-0.03	3.27	0.96	3
4-OH-BDE-42	6.50	219.21	233.25	2.59	-6.64	-1.67	0.22	-0.20	0.06	3.47	0.96	4
4'-OH-BDE-49	6.50	225.41	235.43	2.85	-6.67	-1.63	0.23	-0.18	0.06	3.42	0.98	4
3-OH-BDE-47	6.50	173.94	238.90	2.92	-6.65	-1.47	0.23	-0.12	0.10	3.18	0.99	4
5-OH-BDE-47*	6.50	271.60	236.23	1.80	-6.52	-1.53	0.22	-0.18	0.07	3.25	0.97	4
6-OH-BDE-47*	6.50	208.27	237.07	3.33	-6.60	-1.49	0.26	-0.21	0.06	3.20	0.97	4
4-OH-BDE-90	7.33	247.79	258.19	2.11	-6.70	-1.93	0.23	-0.13	0.07	3.90	0.98	5
6-OH-BDE-85	7.33	236.70	256.94	3.39	-6.65	-1.92	0.26	-0.21	0.08	3.89	0.95	5
6-OH-BDE-87*	7.33	184.58	254.48	2.83	-6.69	-1.90	0.26	-0.21	0.08	3.85	0.95	5
6-OH-BDE-82	7.33	237.33	254.96	3.98	-6.78	-1.90	0.25	-0.21	0.08	3.86	0.94	5
6'-OH-BDE-99	7.33	198.03	255.71	0.49	-6.93	-1.70	0.29	-0.25	-0.01	3.56	0.96	5
5'-OH-BDE-99	7.33	210.78	257.00	1.97	-6.81	-1.70	0.26	-0.18	0.06	3.54	0.97	5
6-OH-BDE-157	8.15	230.38	276.56	3.39	-6.82	-1.97	0.26	-0.22	0.02	3.98	0.93	6
6-OH-BDE-140	8.15	279.94	278.76	3.08	-6.71	-1.84	0.27	-0.17	0.07	3.75	0.95	6
3'-OH-BDE-154	8.15	220.14	277.08	3.11	-6.77	-1.90	0.23	-0.12	0.09	3.86	0.98	6
Minimal	4.84	158.11	193.56	0.49	-6.93	-1.97	0.22	-0.25	-0.03	2.87	0.93	2
Maximal	8.15	279.94	278.76	4.41	-6.43	-1.27	0.29	-0.12	0.1	3.98	0.99	6
Mean	6.82	216.21	243.93	2.6	-6.67	-1.68	0.25	-0.2	0.06	3.5	0.97	4

^a Compounds marked with asterisk (*) were selected to form the external validation set. ^b a.u., atom unit;

^c a.c.u., atom charge unit.

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Table S2. The determined REC_{20} values for the 18 HO-PBDEs

Compounds ^a	Mean REC_{20} ^a (mol/L)	SD ^b
3'-OH-BDE-7	2.3×10^{-9}	4.1×10^{-10}
4'-OH-BDE-17	2.2×10^{-9}	6.9×10^{-10}
3'-OH-BDE-28	5.3×10^{-8}	4.5×10^{-9}
2'-OH-BDE-28	8.6×10^{-9}	4.3×10^{-10}
4-OH-BDE-42	1.9×10^{-10}	3.3×10^{-11}
4'-OH-BDE-49	1.4×10^{-8}	6.5×10^{-9}
3-OH-BDE-47	1.7×10^{-9}	3.1×10^{-10}
5-OH-BDE-47	3.7×10^{-9}	3.2×10^{-10}
6-OH-BDE-47	3.7×10^{-11}	6.3×10^{-12}
4-OH-BDE-90	2.4×10^{-8}	7.4×10^{-9}
6-OH-BDE-85	1.7×10^{-10}	4.3×10^{-11}
6-OH-BDE-87	5.2×10^{-8}	2.6×10^{-9}
6-OH-BDE-82	3.7×10^{-11}	6.9×10^{-12}
6'-OH-BDE-99	2.4×10^{-10}	5.8×10^{-11}
5'-OH-BDE-99	4.5×10^{-11}	6.5×10^{-12}
6-OH-BDE-157	6.3×10^{-13}	3.1×10^{-14}
6-OH-BDE-140	4.9×10^{-12}	2.5×10^{-13}
3'-OH-BDE-154	1.7×10^{-11}	4.1×10^{-12}

^aThyroid hormone activity is recorded as the concentration of test compound showing 20% of the activity of 10^{-6} M T₃ (REC_{20}). ^b SD is standard deviation.

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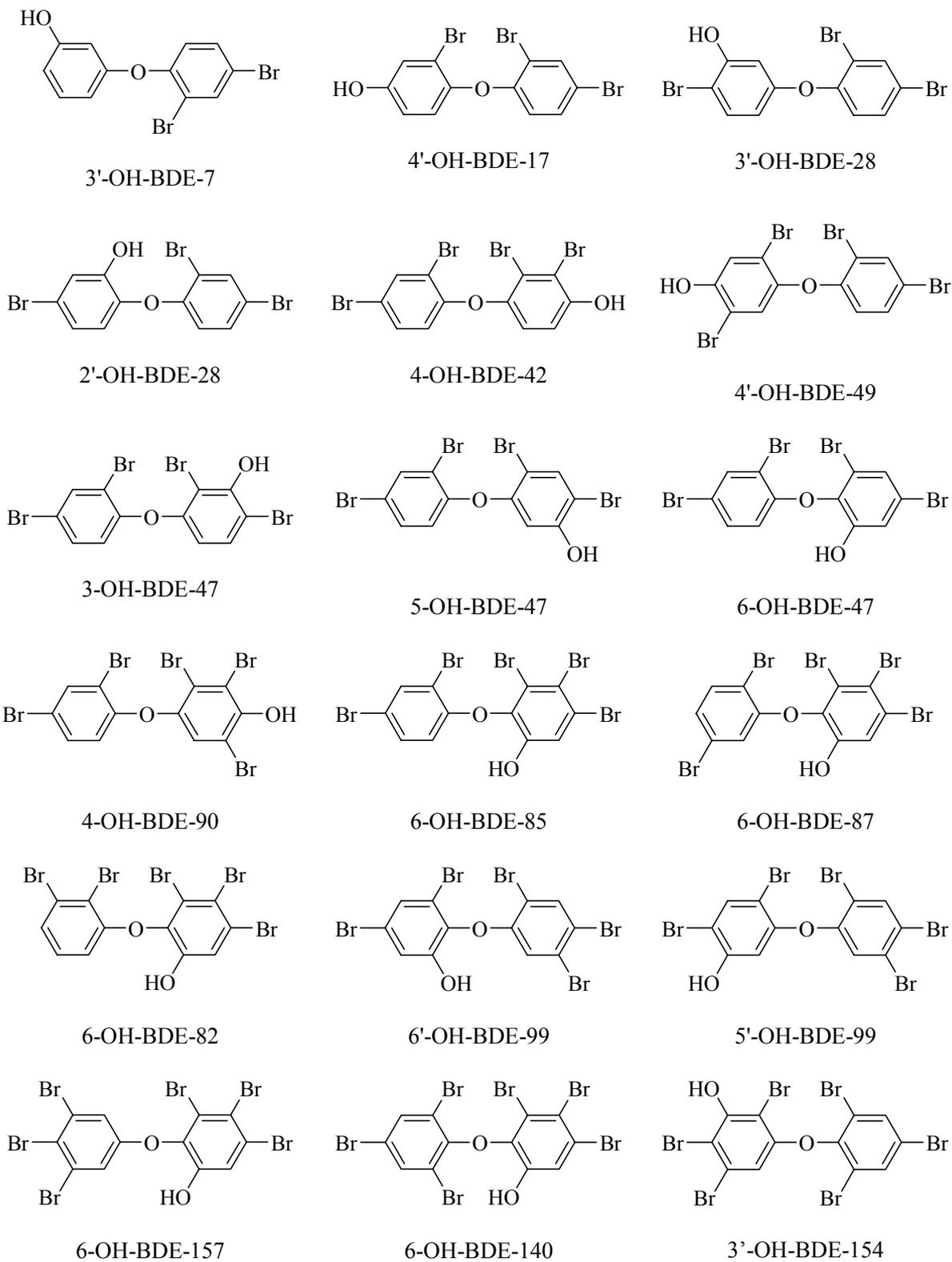


Figure S1. Molecular structures of 18 HO-PBDEs in the current study.

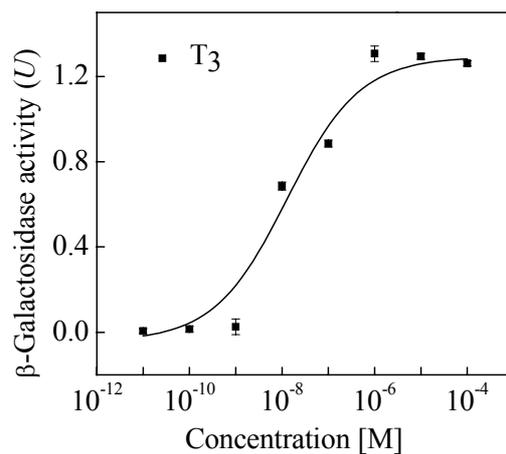


Figure S2. Dose response curves for T₃ in yeast strain human thyroid hormone receptor β (hTR β). U is the activity of β -galactosidase. All the values were determined in triplicate. Error bars indicate the standard deviation (SD).

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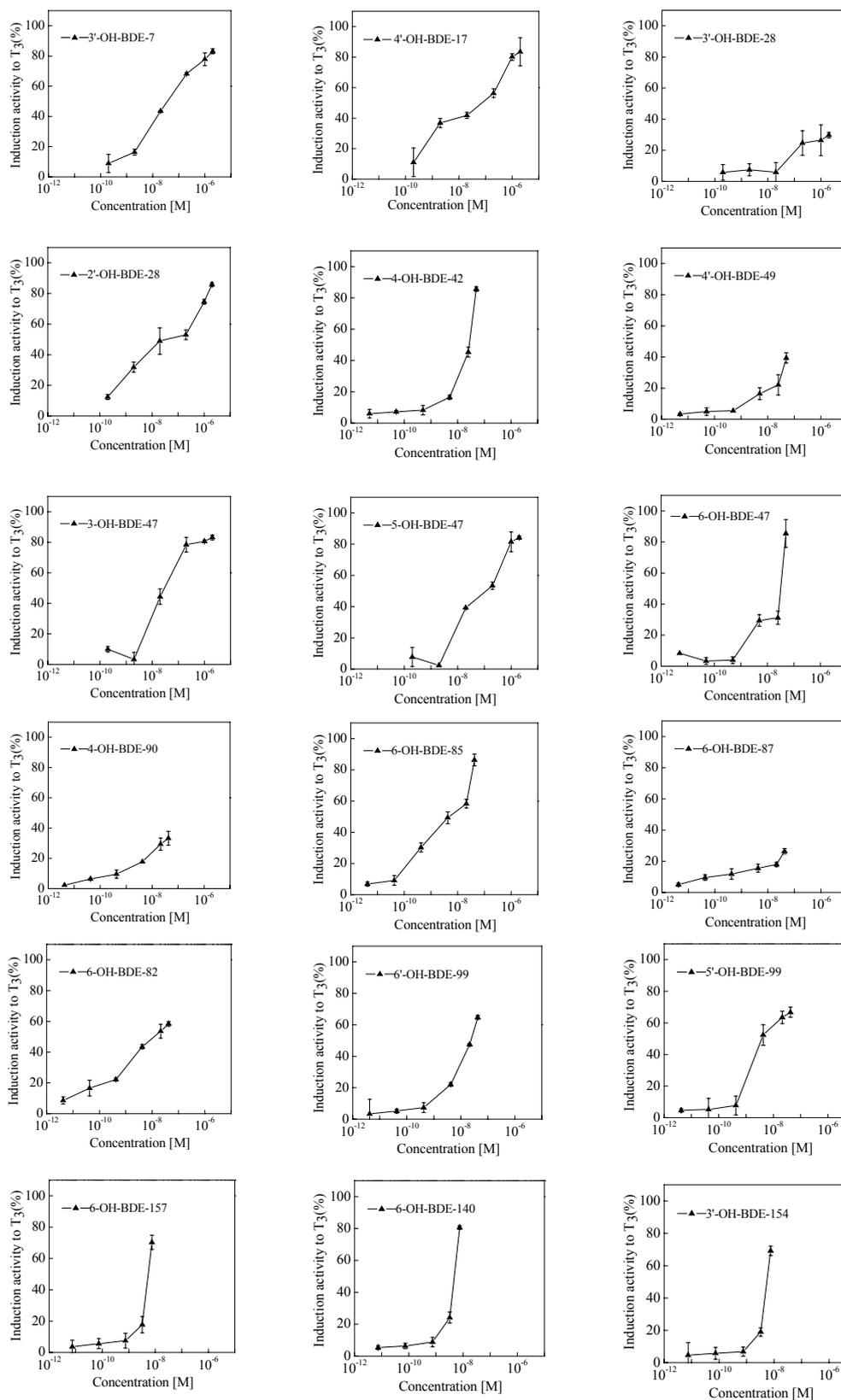


Figure S3. Dose-response relationships for 18 HO-PBDEs determined by the yeast strain hTR β . The induction activity of HO-PBDEs is represented as the percent induction activity relative to the maximum induced by T₃. All the values were determined in triplicate. Error bars indicate the standard deviation (SD).

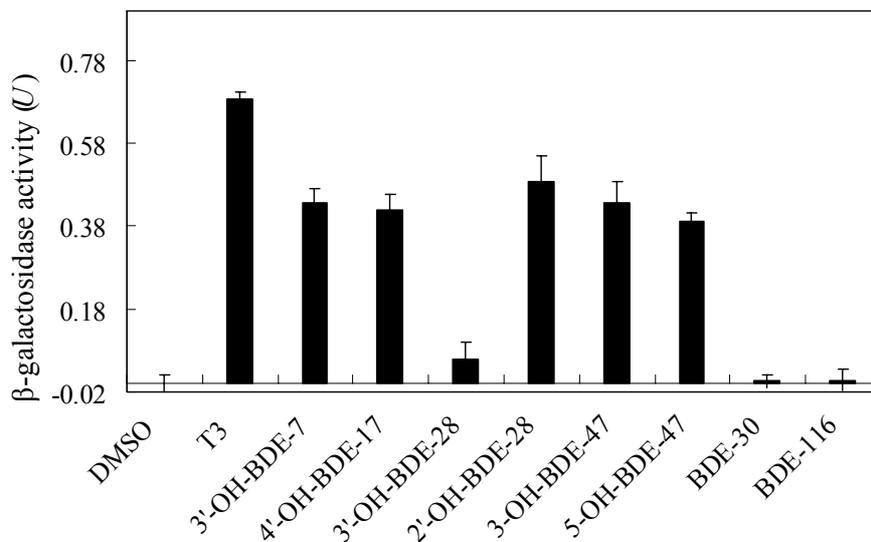


Figure S4. Induction of β -galactosidase activity by the negative control (DMSO), positive control (T_3), representative HO-PBDEs and PBDEs in the recombined yeast assay. The concentration of the tested compounds is 2×10^{-7} mol/L. U is the activity of β -galactosidase. Values are presented as the average \pm standard error ($n = 3$).

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Z-matrices of the optimized structures as well as the energies (*E*) for 18 HO-PBDEs

3'-OH-BDE-7					4'-OH-BDE-17				
C	0	4.76743	-0.83703	-0.48626	C	0	-2.88774	-0.19421	0.38283
C	0	3.59329	-0.16151	-0.82340	C	0	-2.02467	-0.00702	-0.70078
C	0	2.55336	-0.10776	0.09956	C	0	-2.37984	-0.51672	-1.94578
C	0	2.65829	-0.70992	1.34994	C	0	-3.56935	-1.21721	-2.11431
C	0	3.83700	-1.38702	1.66155	C	0	-4.42130	-1.4040	-1.02415
C	0	4.89176	-1.45789	0.7578	C	0	-4.08133	-0.88954	0.22746
O	0	1.44678	0.65002	-0.25631	O	0	-0.88130	0.76031	-0.57609
C	0	0.18622	0.12543	-0.17346	C	0	0.33168	0.15368	-0.38328
C	0	-0.88446	1.01728	-0.03354	C	0	1.46911	0.97150	-0.40661
C	0	-2.19754	0.55716	-0.00635	C	0	2.7364	0.43449	-0.20932
C	0	-2.43981	-0.80793	-0.11676	C	0	2.86721	-0.93314	0.01286
C	0	-1.39242	-1.71111	-0.26076	C	0	1.75251	-1.76129	0.04148
C	0	-0.08410	-1.23932	-0.29263	C	0	0.48771	-1.21364	-0.1566
Br	0	-4.24581	-1.44541	-0.06912	Br	0	4.6128	-1.67671	0.28134
Br	0	-0.55347	2.89017	0.11625	Br	0	1.2900	2.84543	-0.71476
O	0	5.82829	-0.92570	-1.34286	Br	0	-2.44035	0.51606	2.09489
H	0	3.47485	0.32910	-1.78344	O	0	-5.60549	-2.07822	-1.11377
H	0	1.84530	-0.64158	2.06114	H	0	-1.71406	-0.35090	-2.78426
H	0	3.93737	-1.85822	2.63254	H	0	-3.83452	-1.60722	-3.09166
H	0	5.81044	-1.97731	0.99909	H	0	-4.75374	-1.03331	1.06235
H	0	-3.01281	1.25842	0.10372	H	0	3.60420	1.07878	-0.23140
H	0	-1.58862	-2.77101	-0.35458	H	0	1.85970	-2.82305	0.21936
H	0	0.73745	-1.93418	-0.41168	H	0	-0.38453	-1.85393	-0.13049
H	0	5.63627	-0.44854	-2.15698	H	0	-5.75088	-2.37220	-2.01915
<i>E</i> = -5760.98040720 Hartree					<i>E</i> = -8334.51726757 Hartree				
3'-OH-BDE-28					2'-OH-BDE-28				
C	0	-3.67188	0.40543	0.95171	C	0	-3.68235	0.35328	0.99439
C	0	-2.37194	0.84515	1.20891	C	0	-2.37324	0.82327	1.10024
C	0	-1.33527	0.50415	0.3469	C	0	-1.46263	0.56187	0.06993
C	0	-1.56978	-0.27621	-0.78236	C	0	-1.85336	-0.13166	-1.06746
C	0	-2.86613	-0.72051	-1.02979	C	0	-3.15775	-0.60788	-1.1782
C	0	-3.91238	-0.38895	-0.17646	C	0	-4.05238	-0.35872	-0.13967
O	0	-0.09993	1.05322	0.63624	O	0	-0.20097	1.12743	0.22069
C	0	1.05205	0.33604	0.44003	C	0	0.92872	0.34423	0.16172
C	0	2.18611	1.01547	-0.01691	C	0	2.14239	0.98282	-0.11639
C	0	3.40468	0.35467	-0.15275	C	0	3.33263	0.26271	-0.14587
C	0	3.48101	-0.99644	0.16605	C	0	3.3039	-1.10588	0.10206
C	0	2.36518	-1.6905	0.62417	C	0	2.10812	-1.75691	0.38431
C	0	1.15652	-1.01764	0.76432	C	0	0.92363	-1.02686	0.41609
Br	0	5.15291	-1.9095	-0.02833	Br	0	4.93948	-2.09923	0.05272
Br	0	2.07916	2.86827	-0.45522	Br	0	2.18142	2.86055	-0.44999
O	0	-4.71404	0.71705	1.76572	Br	0	-5.84989	-1.00799	-0.2794
Br	0	-5.67748	-1.0126	-0.5444	O	0	-2.00969	1.52624	2.20225
H	0	-2.15628	1.46122	2.07523	H	0	-4.38135	0.55538	1.79465

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<table style="width: 100%; border-collapse: collapse;"> <tr><td>H</td><td>0</td><td>-0.76562</td><td>-0.52561</td><td>-1.46179</td></tr> <tr><td>H</td><td>0</td><td>-3.06916</td><td>-1.32498</td><td>-1.90451</td></tr> <tr><td>H</td><td>0</td><td>4.27367</td><td>0.89155</td><td>-0.50652</td></tr> <tr><td>H</td><td>0</td><td>2.4361</td><td>-2.73955</td><td>0.87917</td></tr> <tr><td>H</td><td>0</td><td>0.28336</td><td>-1.54298</td><td>1.13106</td></tr> <tr><td>H</td><td>0</td><td>-4.40983</td><td>1.2787</td><td>2.48667</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -8334.51857547 Hartree</td></tr> </table>	H	0	-0.76562	-0.52561	-1.46179	H	0	-3.06916	-1.32498	-1.90451	H	0	4.27367	0.89155	-0.50652	H	0	2.4361	-2.73955	0.87917	H	0	0.28336	-1.54298	1.13106	H	0	-4.40983	1.2787	2.48667	<i>E</i> = -8334.51857547 Hartree					<table style="width: 100%; border-collapse: collapse;"> <tr><td>H</td><td>0</td><td>-1.13884</td><td>-0.30033</td><td>-1.86429</td></tr> <tr><td>H</td><td>0</td><td>-3.47033</td><td>-1.15211</td><td>-2.05863</td></tr> <tr><td>H</td><td>0</td><td>4.26324</td><td>0.76787</td><td>-0.36327</td></tr> <tr><td>H</td><td>0</td><td>2.09386</td><td>-2.82021</td><td>0.58387</td></tr> <tr><td>H</td><td>0</td><td>-0.01143</td><td>-1.52393</td><td>0.64084</td></tr> <tr><td>H</td><td>0</td><td>-1.10151</td><td>1.83587</td><td>2.07982</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -8334.52301520 Hartree</td></tr> </table>	H	0	-1.13884	-0.30033	-1.86429	H	0	-3.47033	-1.15211	-2.05863	H	0	4.26324	0.76787	-0.36327	H	0	2.09386	-2.82021	0.58387	H	0	-0.01143	-1.52393	0.64084	H	0	-1.10151	1.83587	2.07982	<i>E</i> = -8334.52301520 Hartree																																																																																																																																																																																																		
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<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">4-OH-BDE-42</td></tr> <tr><td>C</td><td>0</td><td>-3.57801</td><td>0.31073</td><td>0.02673</td></tr> <tr><td>C</td><td>0</td><td>-2.38403</td><td>0.98661</td><td>0.25206</td></tr> <tr><td>C</td><td>0</td><td>-1.1872</td><td>0.28283</td><td>0.43731</td></tr> <tr><td>C</td><td>0</td><td>-1.20713</td><td>-1.11056</td><td>0.39178</td></tr> <tr><td>C</td><td>0</td><td>-2.3982</td><td>-1.7967</td><td>0.16831</td></tr> <tr><td>C</td><td>0</td><td>-3.57461</td><td>-1.08042</td><td>-0.01235</td></tr> <tr><td>O</td><td>0</td><td>-0.05055</td><td>1.0228</td><td>0.63923</td></tr> <tr><td>C</td><td>0</td><td>1.12715</td><td>0.39718</td><td>0.99854</td></tr> <tr><td>C</td><td>0</td><td>2.12086</td><td>0.16481</td><td>0.04311</td></tr> <tr><td>C</td><td>0</td><td>3.34428</td><td>-0.38376</td><td>0.44906</td></tr> <tr><td>C</td><td>0</td><td>3.57642</td><td>-0.69628</td><td>1.79726</td></tr> <tr><td>C</td><td>0</td><td>2.57103</td><td>-0.45164</td><td>2.73498</td></tr> <tr><td>C</td><td>0</td><td>1.36186</td><td>0.09332</td><td>2.33708</td></tr> <tr><td>O</td><td>0</td><td>4.73768</td><td>-1.22628</td><td>2.24756</td></tr> <tr><td>Br</td><td>0</td><td>1.77297</td><td>0.61066</td><td>-1.77018</td></tr> <tr><td>Br</td><td>0</td><td>-5.22075</td><td>-2.01151</td><td>-0.31766</td></tr> <tr><td>Br</td><td>0</td><td>-2.39019</td><td>2.89276</td><td>0.3117</td></tr> <tr><td>Br</td><td>0</td><td>4.76219</td><td>-0.72819</td><td>-0.78747</td></tr> <tr><td>H</td><td>0</td><td>-4.49388</td><td>0.86759</td><td>-0.11332</td></tr> <tr><td>H</td><td>0</td><td>-0.28669</td><td>-1.66343</td><td>0.52851</td></tr> <tr><td>H</td><td>0</td><td>-2.40062</td><td>-2.87804</td><td>0.13327</td></tr> <tr><td>H</td><td>0</td><td>2.76698</td><td>-0.68908</td><td>3.77282</td></tr> <tr><td>H</td><td>0</td><td>0.58302</td><td>0.29982</td><td>3.06086</td></tr> <tr><td>H</td><td>0</td><td>5.35187</td><td>-1.3359</td><td>1.50666</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -10908.0551987 Hartree</td></tr> </table>	4-OH-BDE-42					C	0	-3.57801	0.31073	0.02673	C	0	-2.38403	0.98661	0.25206	C	0	-1.1872	0.28283	0.43731	C	0	-1.20713	-1.11056	0.39178	C	0	-2.3982	-1.7967	0.16831	C	0	-3.57461	-1.08042	-0.01235	O	0	-0.05055	1.0228	0.63923	C	0	1.12715	0.39718	0.99854	C	0	2.12086	0.16481	0.04311	C	0	3.34428	-0.38376	0.44906	C	0	3.57642	-0.69628	1.79726	C	0	2.57103	-0.45164	2.73498	C	0	1.36186	0.09332	2.33708	O	0	4.73768	-1.22628	2.24756	Br	0	1.77297	0.61066	-1.77018	Br	0	-5.22075	-2.01151	-0.31766	Br	0	-2.39019	2.89276	0.3117	Br	0	4.76219	-0.72819	-0.78747	H	0	-4.49388	0.86759	-0.11332	H	0	-0.28669	-1.66343	0.52851	H	0	-2.40062	-2.87804	0.13327	H	0	2.76698	-0.68908	3.77282	H	0	0.58302	0.29982	3.06086	H	0	5.35187	-1.3359	1.50666	<i>E</i> = -10908.0551987 Hartree					<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">4-OH-BDE-49</td></tr> <tr><td>C</td><td>0</td><td>3.20622</td><td>1.06016</td><td>-1.29573</td></tr> <tr><td>C</td><td>0</td><td>1.92822</td><td>1.31115</td><td>-0.81334</td></tr> <tr><td>C</td><td>0</td><td>1.36986</td><td>0.49323</td><td>0.17372</td></tr> <tr><td>C</td><td>0</td><td>2.11134</td><td>-0.57025</td><td>0.67941</td></tr> <tr><td>C</td><td>0</td><td>3.38674</td><td>-0.82004</td><td>0.19213</td></tr> <tr><td>C</td><td>0</td><td>3.95359</td><td>-0.01088</td><td>-0.80078</td></tr> <tr><td>O</td><td>0</td><td>0.13983</td><td>0.77974</td><td>0.72889</td></tr> <tr><td>C</td><td>0</td><td>-0.98606</td><td>0.14533</td><td>0.26685</td></tr> <tr><td>C</td><td>0</td><td>-2.1846</td><td>0.3944</td><td>0.94732</td></tr> <tr><td>C</td><td>0</td><td>-3.37134</td><td>-0.20231</td><td>0.53638</td></tr> <tr><td>C</td><td>0</td><td>-3.35787</td><td>-1.05612</td><td>-0.56263</td></tr> <tr><td>C</td><td>0</td><td>-2.17931</td><td>-1.3163</td><td>-1.25004</td></tr> <tr><td>C</td><td>0</td><td>-0.99587</td><td>-0.71335</td><td>-0.83134</td></tr> <tr><td>Br</td><td>0</td><td>-4.99213</td><td>-1.88037</td><td>-1.12787</td></tr> <tr><td>Br</td><td>0</td><td>-2.20164</td><td>1.55835</td><td>2.45769</td></tr> <tr><td>O</td><td>0</td><td>5.19171</td><td>-0.20263</td><td>-1.3125</td></tr> <tr><td>Br</td><td>0</td><td>0.94429</td><td>2.78943</td><td>-1.5007</td></tr> <tr><td>Br</td><td>0</td><td>4.41143</td><td>-2.28324</td><td>0.88798</td></tr> <tr><td>H</td><td>0</td><td>3.64669</td><td>1.68964</td><td>-2.05732</td></tr> <tr><td>H</td><td>0</td><td>1.68224</td><td>-1.18813</td><td>1.45737</td></tr> <tr><td>H</td><td>0</td><td>-4.28889</td><td>-0.00113</td><td>1.07143</td></tr> <tr><td>H</td><td>0</td><td>-2.17517</td><td>-1.97876</td><td>-2.10536</td></tr> <tr><td>H</td><td>0</td><td>-0.07574</td><td>-0.91007</td><td>-1.36629</td></tr> <tr><td>H</td><td>0</td><td>5.60479</td><td>-0.96447</td><td>-0.88104</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -10908.0593880 Hartree</td></tr> </table>	4-OH-BDE-49					C	0	3.20622	1.06016	-1.29573	C	0	1.92822	1.31115	-0.81334	C	0	1.36986	0.49323	0.17372	C	0	2.11134	-0.57025	0.67941	C	0	3.38674	-0.82004	0.19213	C	0	3.95359	-0.01088	-0.80078	O	0	0.13983	0.77974	0.72889	C	0	-0.98606	0.14533	0.26685	C	0	-2.1846	0.3944	0.94732	C	0	-3.37134	-0.20231	0.53638	C	0	-3.35787	-1.05612	-0.56263	C	0	-2.17931	-1.3163	-1.25004	C	0	-0.99587	-0.71335	-0.83134	Br	0	-4.99213	-1.88037	-1.12787	Br	0	-2.20164	1.55835	2.45769	O	0	5.19171	-0.20263	-1.3125	Br	0	0.94429	2.78943	-1.5007	Br	0	4.41143	-2.28324	0.88798	H	0	3.64669	1.68964	-2.05732	H	0	1.68224	-1.18813	1.45737	H	0	-4.28889	-0.00113	1.07143	H	0	-2.17517	-1.97876	-2.10536	H	0	-0.07574	-0.91007	-1.36629	H	0	5.60479	-0.96447	-0.88104	<i>E</i> = -10908.0593880 Hartree				
4-OH-BDE-42																																																																																																																																																																																																																																																																					
C	0	-3.57801	0.31073	0.02673																																																																																																																																																																																																																																																																	
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C	0	2.57103	-0.45164	2.73498																																																																																																																																																																																																																																																																	
C	0	1.36186	0.09332	2.33708																																																																																																																																																																																																																																																																	
O	0	4.73768	-1.22628	2.24756																																																																																																																																																																																																																																																																	
Br	0	1.77297	0.61066	-1.77018																																																																																																																																																																																																																																																																	
Br	0	-5.22075	-2.01151	-0.31766																																																																																																																																																																																																																																																																	
Br	0	-2.39019	2.89276	0.3117																																																																																																																																																																																																																																																																	
Br	0	4.76219	-0.72819	-0.78747																																																																																																																																																																																																																																																																	
H	0	-4.49388	0.86759	-0.11332																																																																																																																																																																																																																																																																	
H	0	-0.28669	-1.66343	0.52851																																																																																																																																																																																																																																																																	
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C	0	1.36986	0.49323	0.17372																																																																																																																																																																																																																																																																	
C	0	2.11134	-0.57025	0.67941																																																																																																																																																																																																																																																																	
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C	0	3.95359	-0.01088	-0.80078																																																																																																																																																																																																																																																																	
O	0	0.13983	0.77974	0.72889																																																																																																																																																																																																																																																																	
C	0	-0.98606	0.14533	0.26685																																																																																																																																																																																																																																																																	
C	0	-2.1846	0.3944	0.94732																																																																																																																																																																																																																																																																	
C	0	-3.37134	-0.20231	0.53638																																																																																																																																																																																																																																																																	
C	0	-3.35787	-1.05612	-0.56263																																																																																																																																																																																																																																																																	
C	0	-2.17931	-1.3163	-1.25004																																																																																																																																																																																																																																																																	
C	0	-0.99587	-0.71335	-0.83134																																																																																																																																																																																																																																																																	
Br	0	-4.99213	-1.88037	-1.12787																																																																																																																																																																																																																																																																	
Br	0	-2.20164	1.55835	2.45769																																																																																																																																																																																																																																																																	
O	0	5.19171	-0.20263	-1.3125																																																																																																																																																																																																																																																																	
Br	0	0.94429	2.78943	-1.5007																																																																																																																																																																																																																																																																	
Br	0	4.41143	-2.28324	0.88798																																																																																																																																																																																																																																																																	
H	0	3.64669	1.68964	-2.05732																																																																																																																																																																																																																																																																	
H	0	1.68224	-1.18813	1.45737																																																																																																																																																																																																																																																																	
H	0	-4.28889	-0.00113	1.07143																																																																																																																																																																																																																																																																	
H	0	-2.17517	-1.97876	-2.10536																																																																																																																																																																																																																																																																	
H	0	-0.07574	-0.91007	-1.36629																																																																																																																																																																																																																																																																	
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<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">3'-OH-BDE-47</td></tr> <tr><td>C</td><td>0</td><td>-2.7695</td><td>-0.55587</td><td>-2.34868</td></tr> <tr><td>C</td><td>0</td><td>-1.96857</td><td>0.4874</td><td>-1.8888</td></tr> <tr><td>C</td><td>0</td><td>-0.57898</td><td>0.43214</td><td>-2.03099</td></tr> <tr><td>C</td><td>0</td><td>0.00099</td><td>-0.67846</td><td>-2.64492</td></tr> <tr><td>C</td><td>0</td><td>-0.78709</td><td>-1.72945</td><td>-3.09953</td></tr> <tr><td>C</td><td>0</td><td>-2.16876</td><td>-1.65778</td><td>-2.94657</td></tr> <tr><td>O</td><td>0</td><td>0.1641</td><td>1.51898</td><td>-1.64019</td></tr> <tr><td>C</td><td>0</td><td>1.34917</td><td>1.34786</td><td>-0.96781</td></tr> <tr><td>C</td><td>0</td><td>2.39297</td><td>2.22737</td><td>-1.26657</td></tr> <tr><td>C</td><td>0</td><td>3.60175</td><td>2.15712</td><td>-0.55553</td></tr> <tr><td>C</td><td>0</td><td>3.72698</td><td>1.18127</td><td>0.4426</td></tr> <tr><td>C</td><td>0</td><td>2.69038</td><td>0.30696</td><td>0.73857</td></tr> <tr><td>C</td><td>0</td><td>1.49514</td><td>0.39086</td><td>0.03698</td></tr> <tr><td>Br</td><td>0</td><td>5.38186</td><td>1.07768</td><td>1.41105</td></tr> </table>	3'-OH-BDE-47					C	0	-2.7695	-0.55587	-2.34868	C	0	-1.96857	0.4874	-1.8888	C	0	-0.57898	0.43214	-2.03099	C	0	0.00099	-0.67846	-2.64492	C	0	-0.78709	-1.72945	-3.09953	C	0	-2.16876	-1.65778	-2.94657	O	0	0.1641	1.51898	-1.64019	C	0	1.34917	1.34786	-0.96781	C	0	2.39297	2.22737	-1.26657	C	0	3.60175	2.15712	-0.55553	C	0	3.72698	1.18127	0.4426	C	0	2.69038	0.30696	0.73857	C	0	1.49514	0.39086	0.03698	Br	0	5.38186	1.07768	1.41105	<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">5-OH-BDE-47</td></tr> <tr><td>C</td><td>0</td><td>-3.5232</td><td>0.0681</td><td>0.56602</td></tr> <tr><td>C</td><td>0</td><td>-2.24554</td><td>0.62458</td><td>0.61406</td></tr> <tr><td>C</td><td>0</td><td>-1.35114</td><td>0.43179</td><td>-0.44073</td></tr> <tr><td>C</td><td>0</td><td>-1.74351</td><td>-0.31933</td><td>-1.54721</td></tr> <tr><td>C</td><td>0</td><td>-3.01145</td><td>-0.88581</td><td>-1.60531</td></tr> <tr><td>C</td><td>0</td><td>-3.89018</td><td>-0.68446</td><td>-0.54381</td></tr> <tr><td>O</td><td>0</td><td>-0.12636</td><td>1.06319</td><td>-0.43088</td></tr> <tr><td>C</td><td>0</td><td>1.0258</td><td>0.33854</td><td>-0.27376</td></tr> <tr><td>C</td><td>0</td><td>2.23362</td><td>0.98591</td><td>-0.57135</td></tr> <tr><td>C</td><td>0</td><td>3.43724</td><td>0.31611</td><td>-0.39963</td></tr> <tr><td>C</td><td>0</td><td>3.44088</td><td>-0.99484</td><td>0.06278</td></tr> <tr><td>C</td><td>0</td><td>2.24484</td><td>-1.65398</td><td>0.36348</td></tr> <tr><td>C</td><td>0</td><td>1.03923</td><td>-0.97136</td><td>0.19204</td></tr> <tr><td>Br</td><td>0</td><td>5.10039</td><td>-1.92865</td><td>0.2959</td></tr> </table>	5-OH-BDE-47					C	0	-3.5232	0.0681	0.56602	C	0	-2.24554	0.62458	0.61406	C	0	-1.35114	0.43179	-0.44073	C	0	-1.74351	-0.31933	-1.54721	C	0	-3.01145	-0.88581	-1.60531	C	0	-3.89018	-0.68446	-0.54381	O	0	-0.12636	1.06319	-0.43088	C	0	1.0258	0.33854	-0.27376	C	0	2.23362	0.98591	-0.57135	C	0	3.43724	0.31611	-0.39963	C	0	3.44088	-0.99484	0.06278	C	0	2.24484	-1.65398	0.36348	C	0	1.03923	-0.97136	0.19204	Br	0	5.10039	-1.92865	0.2959																																																																																																														
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Supplemental Material

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border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">4-OH-BDE-90</td></tr> <tr><td>C</td><td>0</td><td>4.00438</td><td>-0.03279</td><td>0.31145</td></tr> <tr><td>C</td><td>0</td><td>2.80284</td><td>-0.32339</td><td>0.94858</td></tr> <tr><td>C</td><td>0</td><td>1.58053</td><td>-0.10504</td><td>0.30119</td></tr> <tr><td>C</td><td>0</td><td>1.58065</td><td>0.40582</td><td>-0.99594</td></tr> <tr><td>C</td><td>0</td><td>2.77851</td><td>0.70167</td><td>-1.64128</td></tr> <tr><td>C</td><td>0</td><td>3.98128</td><td>0.48068</td><td>-0.98175</td></tr> <tr><td>O</td><td>0</td><td>0.43888</td><td>-0.44279</td><td>0.98527</td></tr> <tr><td>C</td><td>0</td><td>-0.79002</td><td>-0.00777</td><td>0.53854</td></tr> <tr><td>C</td><td>0</td><td>-1.69308</td><td>-0.92002</td><td>-0.01391</td></tr> <tr><td>C</td><td>0</td><td>-2.97248</td><td>-0.47504</td><td>-0.36602</td></tr> <tr><td>C</td><td>0</td><td>-3.36187</td><td>0.86233</td><td>-0.1814</td></tr> <tr><td>C</td><td>0</td><td>-2.42951</td><td>1.74957</td><td>0.37464</td></tr> <tr><td>C</td><td>0</td><td>-1.16354</td><td>1.31786</td><td>0.73557</td></tr> <tr><td>O</td><td>0</td><td>-4.58243</td><td>1.32748</td><td>-0.51078</td></tr> <tr><td>Br</td><td>0</td><td>-1.14891</td><td>-2.72153</td><td>-0.2549</td></tr> <tr><td>Br</td><td>0</td><td>5.6358</td><td>0.88798</td><td>-1.85579</td></tr> <tr><td>Br</td><td>0</td><td>2.83393</td><td>-1.02421</td><td>2.72139</td></tr> <tr><td>Br</td><td>0</td><td>-4.27519</td><td>-1.65515</td><td>-1.11897</td></tr> <tr><td>Br</td><td>0</td><td>-2.91807</td><td>3.56801</td><td>0.6525</td></tr> <tr><td>H</td><td>0</td><td>4.94075</td><td>-0.20349</td><td>0.82395</td></tr> <tr><td>H</td><td>0</td><td>0.64114</td><td>0.57104</td><td>-1.50757</td></tr> <tr><td>H</td><td>0</td><td>2.7668</td><td>1.0959</td><td>-2.64874</td></tr> <tr><td>H</td><td>0</td><td>-0.45598</td><td>2.00429</td><td>1.18136</td></tr> <tr><td>H</td><td>0</td><td>-5.11551</td><td>0.60268</td><td>-0.87105</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -13481.5916412 Hartree</td></tr> </table>	4-OH-BDE-90					C	0	4.00438	-0.03279	0.31145	C	0	2.80284	-0.32339	0.94858	C	0	1.58053	-0.10504	0.30119	C	0	1.58065	0.40582	-0.99594	C	0	2.77851	0.70167	-1.64128	C	0	3.98128	0.48068	-0.98175	O	0	0.43888	-0.44279	0.98527	C	0	-0.79002	-0.00777	0.53854	C	0	-1.69308	-0.92002	-0.01391	C	0	-2.97248	-0.47504	-0.36602	C	0	-3.36187	0.86233	-0.1814	C	0	-2.42951	1.74957	0.37464	C	0	-1.16354	1.31786	0.73557	O	0	-4.58243	1.32748	-0.51078	Br	0	-1.14891	-2.72153	-0.2549	Br	0	5.6358	0.88798	-1.85579	Br	0	2.83393	-1.02421	2.72139	Br	0	-4.27519	-1.65515	-1.11897	Br	0	-2.91807	3.56801	0.6525	H	0	4.94075	-0.20349	0.82395	H	0	0.64114	0.57104	-1.50757	H	0	2.7668	1.0959	-2.64874	H	0	-0.45598	2.00429	1.18136	H	0	-5.11551	0.60268	-0.87105	<i>E</i> = -13481.5916412 Hartree				
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O	0	-0.00263	0.95973	-0.38598																																																																																																																																																																																																																																																																	
C	0	1.23234	0.36405	-0.33798																																																																																																																																																																																																																																																																	
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H	0	-2.28803	-2.69343	1.16336																																																																																																																																																																																																																																																																	
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C	0	1.58065	0.40582	-0.99594																																																																																																																																																																																																																																																																	
C	0	2.77851	0.70167	-1.64128																																																																																																																																																																																																																																																																	
C	0	3.98128	0.48068	-0.98175																																																																																																																																																																																																																																																																	
O	0	0.43888	-0.44279	0.98527																																																																																																																																																																																																																																																																	
C	0	-0.79002	-0.00777	0.53854																																																																																																																																																																																																																																																																	
C	0	-1.69308	-0.92002	-0.01391																																																																																																																																																																																																																																																																	
C	0	-2.97248	-0.47504	-0.36602																																																																																																																																																																																																																																																																	
C	0	-3.36187	0.86233	-0.1814																																																																																																																																																																																																																																																																	
C	0	-2.42951	1.74957	0.37464																																																																																																																																																																																																																																																																	
C	0	-1.16354	1.31786	0.73557																																																																																																																																																																																																																																																																	
O	0	-4.58243	1.32748	-0.51078																																																																																																																																																																																																																																																																	
Br	0	-1.14891	-2.72153	-0.2549																																																																																																																																																																																																																																																																	
Br	0	5.6358	0.88798	-1.85579																																																																																																																																																																																																																																																																	
Br	0	2.83393	-1.02421	2.72139																																																																																																																																																																																																																																																																	
Br	0	-4.27519	-1.65515	-1.11897																																																																																																																																																																																																																																																																	
Br	0	-2.91807	3.56801	0.6525																																																																																																																																																																																																																																																																	
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H	0	0.64114	0.57104	-1.50757																																																																																																																																																																																																																																																																	
H	0	2.7668	1.0959	-2.64874																																																																																																																																																																																																																																																																	
H	0	-0.45598	2.00429	1.18136																																																																																																																																																																																																																																																																	
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C	0	-0.61628	0.17291	0.72347																																																																																																																																																																																																																																																																	
C	0	-1.57536	0.58804	-0.20366																																																																																																																																																																																																																																																																	
C	0	-2.87115	0.03963	-0.19533																																																																																																																																																																																																																																																																	
6-OH-BDE-87																																																																																																																																																																																																																																																																					
C	0	-4.52683	-0.17835	0.146544																																																																																																																																																																																																																																																																	
C	0	-3.38908	-0.94165	0.378953																																																																																																																																																																																																																																																																	
C	0	-2.12247	-0.35529	0.280549																																																																																																																																																																																																																																																																	
C	0	-2.00746	0.992623	-0.05551																																																																																																																																																																																																																																																																	
C	0	-3.15902	1.738188	-0.27907																																																																																																																																																																																																																																																																	
C	0	-4.42385	1.171739	-0.18319																																																																																																																																																																																																																																																																	
O	0	-1.03412	-1.16573	0.491317																																																																																																																																																																																																																																																																	
C	0	0.212607	-0.61888	0.660595																																																																																																																																																																																																																																																																	
C	0	1.174292	-0.7163	-0.34792																																																																																																																																																																																																																																																																	
C	0	2.485783	-0.25138	-0.13989																																																																																																																																																																																																																																																																	

Supplemental Material

<table style="width: 100%; border-collapse: collapse;"> <tr><td>C</td><td>0</td><td>-3.17115</td><td>-0.93432</td><td>0.76287</td></tr> <tr><td>C</td><td>0</td><td>-2.21841</td><td>-1.34969</td><td>1.68954</td></tr> <tr><td>C</td><td>0</td><td>-0.94345</td><td>-0.79753</td><td>1.68109</td></tr> <tr><td>Br</td><td>0</td><td>-4.88964</td><td>-1.75627</td><td>0.87518</td></tr> <tr><td>Br</td><td>0</td><td>-1.0551</td><td>1.91661</td><td>-1.4575</td></tr> <tr><td>Br</td><td>0</td><td>5.70063</td><td>-1.86601</td><td>-1.196</td></tr> <tr><td>Br</td><td>0</td><td>3.06714</td><td>2.25517</td><td>1.72773</td></tr> <tr><td>Br</td><td>0</td><td>-4.17654</td><td>0.6095</td><td>-1.4534</td></tr> <tr><td>O</td><td>0</td><td>0.02889</td><td>-1.14613</td><td>2.56153</td></tr> <tr><td>H</td><td>0</td><td>5.10338</td><td>0.53116</td><td>0.46448</td></tr> <tr><td>H</td><td>0</td><td>0.72275</td><td>-1.44363</td><td>-0.72941</td></tr> <tr><td>H</td><td>0</td><td>2.80522</td><td>-2.5049</td><td>-1.52971</td></tr> <tr><td>H</td><td>0</td><td>-2.48017</td><td>-2.10001</td><td>2.42571</td></tr> <tr><td>H</td><td>0</td><td>-0.29967</td><td>-1.80923</td><td>3.17842</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -13481.5840630 Hartree</td></tr> </table>	C	0	-3.17115	-0.93432	0.76287	C	0	-2.21841	-1.34969	1.68954	C	0	-0.94345	-0.79753	1.68109	Br	0	-4.88964	-1.75627	0.87518	Br	0	-1.0551	1.91661	-1.4575	Br	0	5.70063	-1.86601	-1.196	Br	0	3.06714	2.25517	1.72773	Br	0	-4.17654	0.6095	-1.4534	O	0	0.02889	-1.14613	2.56153	H	0	5.10338	0.53116	0.46448	H	0	0.72275	-1.44363	-0.72941	H	0	2.80522	-2.5049	-1.52971	H	0	-2.48017	-2.10001	2.42571	H	0	-0.29967	-1.80923	3.17842	<i>E</i> = -13481.5840630 Hartree					<table style="width: 100%; border-collapse: collapse;"> <tr><td>C</td><td>0</td><td>2.798812</td><td>0.313197</td><td>1.101225</td></tr> <tr><td>C</td><td>0</td><td>1.843851</td><td>0.408217</td><td>2.110026</td></tr> <tr><td>C</td><td>0</td><td>0.552595</td><td>-0.06022</td><td>1.900583</td></tr> <tr><td>Br</td><td>0</td><td>4.538624</td><td>0.985834</td><td>1.502496</td></tr> <tr><td>Br</td><td>0</td><td>0.635621</td><td>-1.50083</td><td>-1.99154</td></tr> <tr><td>Br</td><td>0</td><td>-3.56033</td><td>-2.78455</td><td>0.833409</td></tr> <tr><td>Br</td><td>0</td><td>3.795207</td><td>-0.38887</td><td>-1.51025</td></tr> <tr><td>O</td><td>0</td><td>-0.42371</td><td>-0.00943</td><td>2.841978</td></tr> <tr><td>Br</td><td>0</td><td>-2.98496</td><td>3.590853</td><td>-0.73524</td></tr> <tr><td>H</td><td>0</td><td>-5.50203</td><td>-0.6411</td><td>0.226698</td></tr> <tr><td>H</td><td>0</td><td>-1.03016</td><td>1.446702</td><td>-0.14554</td></tr> <tr><td>H</td><td>0</td><td>-5.31277</td><td>1.761774</td><td>-0.36002</td></tr> <tr><td>H</td><td>0</td><td>2.115466</td><td>0.842606</td><td>3.06453</td></tr> <tr><td>H</td><td>0</td><td>-0.08872</td><td>0.394854</td><td>3.649769</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -13481.5846054 Hartree</td></tr> </table>	C	0	2.798812	0.313197	1.101225	C	0	1.843851	0.408217	2.110026	C	0	0.552595	-0.06022	1.900583	Br	0	4.538624	0.985834	1.502496	Br	0	0.635621	-1.50083	-1.99154	Br	0	-3.56033	-2.78455	0.833409	Br	0	3.795207	-0.38887	-1.51025	O	0	-0.42371	-0.00943	2.841978	Br	0	-2.98496	3.590853	-0.73524	H	0	-5.50203	-0.6411	0.226698	H	0	-1.03016	1.446702	-0.14554	H	0	-5.31277	1.761774	-0.36002	H	0	2.115466	0.842606	3.06453	H	0	-0.08872	0.394854	3.649769	<i>E</i> = -13481.5846054 Hartree																																																																																																																		
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C	0	-2.21841	-1.34969	1.68954																																																																																																																																																																																																																																																																	
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<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">6-OH-BDE-82</td></tr> <tr><td>C</td><td>0</td><td>-4.01773</td><td>-0.40733</td><td>0.92195</td></tr> <tr><td>C</td><td>0</td><td>-3.01081</td><td>-0.15686</td><td>-0.01419</td></tr> <tr><td>C</td><td>0</td><td>-1.67074</td><td>-0.2938</td><td>0.38288</td></tr> <tr><td>C</td><td>0</td><td>-1.35254</td><td>-0.66542</td><td>1.68482</td></tr> <tr><td>C</td><td>0</td><td>-2.371</td><td>-0.91245</td><td>2.59924</td></tr> <tr><td>C</td><td>0</td><td>-3.70305</td><td>-0.78668</td><td>2.22674</td></tr> <tr><td>O</td><td>0</td><td>-0.71612</td><td>-0.00578</td><td>-0.56491</td></tr> <tr><td>C</td><td>0</td><td>0.58608</td><td>-0.38549</td><td>-0.36951</td></tr> <tr><td>C</td><td>0</td><td>1.5699</td><td>0.56894</td><td>-0.09952</td></tr> <tr><td>C</td><td>0</td><td>2.92484</td><td>0.20112</td><td>-0.00532</td></tr> <tr><td>C</td><td>0</td><td>3.2595</td><td>-1.14498</td><td>-0.18514</td></tr> <tr><td>C</td><td>0</td><td>2.28219</td><td>-2.09882</td><td>-0.45743</td></tr> <tr><td>C</td><td>0</td><td>0.94721</td><td>-1.72733</td><td>-0.55811</td></tr> <tr><td>Br</td><td>0</td><td>5.05956</td><td>-1.76879</td><td>-0.07752</td></tr> <tr><td>Br</td><td>0</td><td>1.00002</td><td>2.3668</td><td>0.12566</td></tr> <tr><td>Br</td><td>0</td><td>-3.38268</td><td>0.35893</td><td>-1.80492</td></tr> <tr><td>Br</td><td>0</td><td>4.2627</td><td>1.50181</td><td>0.35684</td></tr> <tr><td>O</td><td>0</td><td>-0.05349</td><td>-2.60171</td><td>-0.83417</td></tr> <tr><td>Br</td><td>0</td><td>-5.86651</td><td>-0.2511</td><td>0.47024</td></tr> <tr><td>H</td><td>0</td><td>-0.31429</td><td>-0.75284</td><td>1.97806</td></tr> <tr><td>H</td><td>0</td><td>-2.12262</td><td>-1.20076</td><td>3.61367</td></tr> <tr><td>H</td><td>0</td><td>-4.49822</td><td>-0.97651</td><td>2.93462</td></tr> <tr><td>H</td><td>0</td><td>2.56987</td><td>-3.13334</td><td>-0.60101</td></tr> <tr><td>H</td><td>0</td><td>0.30098</td><td>-3.48979</td><td>-0.9516</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -13481.5795644 Hartree</td></tr> </table>	6-OH-BDE-82					C	0	-4.01773	-0.40733	0.92195	C	0	-3.01081	-0.15686	-0.01419	C	0	-1.67074	-0.2938	0.38288	C	0	-1.35254	-0.66542	1.68482	C	0	-2.371	-0.91245	2.59924	C	0	-3.70305	-0.78668	2.22674	O	0	-0.71612	-0.00578	-0.56491	C	0	0.58608	-0.38549	-0.36951	C	0	1.5699	0.56894	-0.09952	C	0	2.92484	0.20112	-0.00532	C	0	3.2595	-1.14498	-0.18514	C	0	2.28219	-2.09882	-0.45743	C	0	0.94721	-1.72733	-0.55811	Br	0	5.05956	-1.76879	-0.07752	Br	0	1.00002	2.3668	0.12566	Br	0	-3.38268	0.35893	-1.80492	Br	0	4.2627	1.50181	0.35684	O	0	-0.05349	-2.60171	-0.83417	Br	0	-5.86651	-0.2511	0.47024	H	0	-0.31429	-0.75284	1.97806	H	0	-2.12262	-1.20076	3.61367	H	0	-4.49822	-0.97651	2.93462	H	0	2.56987	-3.13334	-0.60101	H	0	0.30098	-3.48979	-0.9516	<i>E</i> = -13481.5795644 Hartree					<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">6'-OH-BDE-99</td></tr> <tr><td>C</td><td>0</td><td>-3.50111</td><td>-0.14736</td><td>0.82359</td></tr> <tr><td>C</td><td>0</td><td>-2.25604</td><td>0.47584</td><td>0.80044</td></tr> <tr><td>C</td><td>0</td><td>-1.66407</td><td>0.84041</td><td>-0.40813</td></tr> <tr><td>C</td><td>0</td><td>-2.35301</td><td>0.62899</td><td>-1.61154</td></tr> <tr><td>C</td><td>0</td><td>-3.60015</td><td>0.00653</td><td>-1.60514</td></tr> <tr><td>C</td><td>0</td><td>-4.1476</td><td>-0.37686</td><td>-0.38835</td></tr> <tr><td>O</td><td>0</td><td>-0.4629</td><td>1.52326</td><td>-0.49351</td></tr> <tr><td>C</td><td>0</td><td>0.73237</td><td>0.8474</td><td>-0.36611</td></tr> <tr><td>C</td><td>0</td><td>1.90022</td><td>1.61628</td><td>-0.33474</td></tr> <tr><td>C</td><td>0</td><td>3.13681</td><td>0.99671</td><td>-0.22495</td></tr> <tr><td>C</td><td>0</td><td>3.22919</td><td>-0.39336</td><td>-0.14754</td></tr> <tr><td>C</td><td>0</td><td>2.06402</td><td>-1.16112</td><td>-0.1871</td></tr> <tr><td>C</td><td>0</td><td>0.82161</td><td>-0.53801</td><td>-0.29824</td></tr> <tr><td>Br</td><td>0</td><td>4.96553</td><td>-1.16293</td><td>0.00981</td></tr> <tr><td>Br</td><td>0</td><td>1.80508</td><td>3.51514</td><td>-0.44948</td></tr> <tr><td>Br</td><td>0</td><td>-1.36861</td><td>0.84496</td><td>2.4457</td></tr> <tr><td>O</td><td>0</td><td>-1.82297</td><td>1.01962</td><td>-2.79532</td></tr> <tr><td>Br</td><td>0</td><td>-5.85768</td><td>-1.23441</td><td>-0.37082</td></tr> <tr><td>Br</td><td>0</td><td>2.09141</td><td>-3.06349</td><td>-0.09444</td></tr> <tr><td>H</td><td>0</td><td>-3.95286</td><td>-0.4338</td><td>1.76192</td></tr> <tr><td>H</td><td>0</td><td>-4.11583</td><td>-0.15563</td><td>-2.54154</td></tr> <tr><td>H</td><td>0</td><td>4.03594</td><td>1.59648</td><td>-0.19814</td></tr> <tr><td>H</td><td>0</td><td>-0.0779</td><td>-1.13769</td><td>-0.32734</td></tr> <tr><td>H</td><td>0</td><td>-1.02616</td><td>1.54055</td><td>-2.62438</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -13481.5951554 Hartree</td></tr> </table>	6'-OH-BDE-99					C	0	-3.50111	-0.14736	0.82359	C	0	-2.25604	0.47584	0.80044	C	0	-1.66407	0.84041	-0.40813	C	0	-2.35301	0.62899	-1.61154	C	0	-3.60015	0.00653	-1.60514	C	0	-4.1476	-0.37686	-0.38835	O	0	-0.4629	1.52326	-0.49351	C	0	0.73237	0.8474	-0.36611	C	0	1.90022	1.61628	-0.33474	C	0	3.13681	0.99671	-0.22495	C	0	3.22919	-0.39336	-0.14754	C	0	2.06402	-1.16112	-0.1871	C	0	0.82161	-0.53801	-0.29824	Br	0	4.96553	-1.16293	0.00981	Br	0	1.80508	3.51514	-0.44948	Br	0	-1.36861	0.84496	2.4457	O	0	-1.82297	1.01962	-2.79532	Br	0	-5.85768	-1.23441	-0.37082	Br	0	2.09141	-3.06349	-0.09444	H	0	-3.95286	-0.4338	1.76192	H	0	-4.11583	-0.15563	-2.54154	H	0	4.03594	1.59648	-0.19814	H	0	-0.0779	-1.13769	-0.32734	H	0	-1.02616	1.54055	-2.62438	<i>E</i> = -13481.5951554 Hartree				
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C	0	-2.371	-0.91245	2.59924																																																																																																																																																																																																																																																																	
C	0	-3.70305	-0.78668	2.22674																																																																																																																																																																																																																																																																	
O	0	-0.71612	-0.00578	-0.56491																																																																																																																																																																																																																																																																	
C	0	0.58608	-0.38549	-0.36951																																																																																																																																																																																																																																																																	
C	0	1.5699	0.56894	-0.09952																																																																																																																																																																																																																																																																	
C	0	2.92484	0.20112	-0.00532																																																																																																																																																																																																																																																																	
C	0	3.2595	-1.14498	-0.18514																																																																																																																																																																																																																																																																	
C	0	2.28219	-2.09882	-0.45743																																																																																																																																																																																																																																																																	
C	0	0.94721	-1.72733	-0.55811																																																																																																																																																																																																																																																																	
Br	0	5.05956	-1.76879	-0.07752																																																																																																																																																																																																																																																																	
Br	0	1.00002	2.3668	0.12566																																																																																																																																																																																																																																																																	
Br	0	-3.38268	0.35893	-1.80492																																																																																																																																																																																																																																																																	
Br	0	4.2627	1.50181	0.35684																																																																																																																																																																																																																																																																	
O	0	-0.05349	-2.60171	-0.83417																																																																																																																																																																																																																																																																	
Br	0	-5.86651	-0.2511	0.47024																																																																																																																																																																																																																																																																	
H	0	-0.31429	-0.75284	1.97806																																																																																																																																																																																																																																																																	
H	0	-2.12262	-1.20076	3.61367																																																																																																																																																																																																																																																																	
H	0	-4.49822	-0.97651	2.93462																																																																																																																																																																																																																																																																	
H	0	2.56987	-3.13334	-0.60101																																																																																																																																																																																																																																																																	
H	0	0.30098	-3.48979	-0.9516																																																																																																																																																																																																																																																																	
<i>E</i> = -13481.5795644 Hartree																																																																																																																																																																																																																																																																					
6'-OH-BDE-99																																																																																																																																																																																																																																																																					
C	0	-3.50111	-0.14736	0.82359																																																																																																																																																																																																																																																																	
C	0	-2.25604	0.47584	0.80044																																																																																																																																																																																																																																																																	
C	0	-1.66407	0.84041	-0.40813																																																																																																																																																																																																																																																																	
C	0	-2.35301	0.62899	-1.61154																																																																																																																																																																																																																																																																	
C	0	-3.60015	0.00653	-1.60514																																																																																																																																																																																																																																																																	
C	0	-4.1476	-0.37686	-0.38835																																																																																																																																																																																																																																																																	
O	0	-0.4629	1.52326	-0.49351																																																																																																																																																																																																																																																																	
C	0	0.73237	0.8474	-0.36611																																																																																																																																																																																																																																																																	
C	0	1.90022	1.61628	-0.33474																																																																																																																																																																																																																																																																	
C	0	3.13681	0.99671	-0.22495																																																																																																																																																																																																																																																																	
C	0	3.22919	-0.39336	-0.14754																																																																																																																																																																																																																																																																	
C	0	2.06402	-1.16112	-0.1871																																																																																																																																																																																																																																																																	
C	0	0.82161	-0.53801	-0.29824																																																																																																																																																																																																																																																																	
Br	0	4.96553	-1.16293	0.00981																																																																																																																																																																																																																																																																	
Br	0	1.80508	3.51514	-0.44948																																																																																																																																																																																																																																																																	
Br	0	-1.36861	0.84496	2.4457																																																																																																																																																																																																																																																																	
O	0	-1.82297	1.01962	-2.79532																																																																																																																																																																																																																																																																	
Br	0	-5.85768	-1.23441	-0.37082																																																																																																																																																																																																																																																																	
Br	0	2.09141	-3.06349	-0.09444																																																																																																																																																																																																																																																																	
H	0	-3.95286	-0.4338	1.76192																																																																																																																																																																																																																																																																	
H	0	-4.11583	-0.15563	-2.54154																																																																																																																																																																																																																																																																	
H	0	4.03594	1.59648	-0.19814																																																																																																																																																																																																																																																																	
H	0	-0.0779	-1.13769	-0.32734																																																																																																																																																																																																																																																																	
H	0	-1.02616	1.54055	-2.62438																																																																																																																																																																																																																																																																	
<i>E</i> = -13481.5951554 Hartree																																																																																																																																																																																																																																																																					
<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">5'-OH-BDE-99</td></tr> <tr><td>C</td><td>0</td><td>-3.53529</td><td>0.09123</td><td>0.79853</td></tr> <tr><td>C</td><td>0</td><td>-2.28997</td><td>0.7165</td><td>0.82526</td></tr> <tr><td>C</td><td>0</td><td>-1.55173</td><td>0.82354</td><td>-0.3525</td></tr> <tr><td>C</td><td>0</td><td>-2.06062</td><td>0.31485</td><td>-1.5441</td></tr> <tr><td>C</td><td>0</td><td>-3.30486</td><td>-0.31358</td><td>-1.57982</td></tr> <tr><td>C</td><td>0</td><td>-4.03901</td><td>-0.42105</td><td>-0.39013</td></tr> </table>	5'-OH-BDE-99					C	0	-3.53529	0.09123	0.79853	C	0	-2.28997	0.7165	0.82526	C	0	-1.55173	0.82354	-0.3525	C	0	-2.06062	0.31485	-1.5441	C	0	-3.30486	-0.31358	-1.57982	C	0	-4.03901	-0.42105	-0.39013	<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">6-OH-BDE-157</td></tr> <tr><td>C</td><td>0</td><td>-3.44183</td><td>-0.93347</td><td>0.55918</td></tr> <tr><td>C</td><td>0</td><td>-2.20949</td><td>-1.48008</td><td>0.88988</td></tr> <tr><td>C</td><td>0</td><td>-1.04827</td><td>-0.77235</td><td>0.59876</td></tr> <tr><td>C</td><td>0</td><td>-1.10899</td><td>0.46822</td><td>-0.02199</td></tr> <tr><td>C</td><td>0</td><td>-2.35323</td><td>1.00521</td><td>-0.34364</td></tr> <tr><td>C</td><td>0</td><td>-3.54369</td><td>0.32256</td><td>-0.06266</td></tr> </table>	6-OH-BDE-157					C	0	-3.44183	-0.93347	0.55918	C	0	-2.20949	-1.48008	0.88988	C	0	-1.04827	-0.77235	0.59876	C	0	-1.10899	0.46822	-0.02199	C	0	-2.35323	1.00521	-0.34364	C	0	-3.54369	0.32256	-0.06266																																																																																																																																																																																														
5'-OH-BDE-99																																																																																																																																																																																																																																																																					
C	0	-3.53529	0.09123	0.79853																																																																																																																																																																																																																																																																	
C	0	-2.28997	0.7165	0.82526																																																																																																																																																																																																																																																																	
C	0	-1.55173	0.82354	-0.3525																																																																																																																																																																																																																																																																	
C	0	-2.06062	0.31485	-1.5441																																																																																																																																																																																																																																																																	
C	0	-3.30486	-0.31358	-1.57982																																																																																																																																																																																																																																																																	
C	0	-4.03901	-0.42105	-0.39013																																																																																																																																																																																																																																																																	
6-OH-BDE-157																																																																																																																																																																																																																																																																					
C	0	-3.44183	-0.93347	0.55918																																																																																																																																																																																																																																																																	
C	0	-2.20949	-1.48008	0.88988																																																																																																																																																																																																																																																																	
C	0	-1.04827	-0.77235	0.59876																																																																																																																																																																																																																																																																	
C	0	-1.10899	0.46822	-0.02199																																																																																																																																																																																																																																																																	
C	0	-2.35323	1.00521	-0.34364																																																																																																																																																																																																																																																																	
C	0	-3.54369	0.32256	-0.06266																																																																																																																																																																																																																																																																	

Supplemental Material

<table style="width: 100%; border-collapse: collapse;"> <tr><td>O</td><td>0</td><td>-0.35729</td><td>1.51418</td><td>-0.38101</td></tr> <tr><td>C</td><td>0</td><td>0.83241</td><td>0.8401</td><td>-0.31178</td></tr> <tr><td>C</td><td>0</td><td>2.00349</td><td>1.58031</td><td>-0.518</td></tr> <tr><td>C</td><td>0</td><td>3.24172</td><td>0.95926</td><td>-0.44787</td></tr> <tr><td>C</td><td>0</td><td>3.33775</td><td>-0.4059</td><td>-0.17397</td></tr> <tr><td>C</td><td>0</td><td>2.17254</td><td>-1.14516</td><td>0.0321</td></tr> <tr><td>C</td><td>0</td><td>0.92746</td><td>-0.52087</td><td>-0.03619</td></tr> <tr><td>Br</td><td>0</td><td>5.07822</td><td>-1.18056</td><td>-0.10126</td></tr> <tr><td>Br</td><td>0</td><td>1.90612</td><td>3.44297</td><td>-0.90118</td></tr> <tr><td>Br</td><td>0</td><td>-1.61969</td><td>1.4227</td><td>2.46257</td></tr> <tr><td>Br</td><td>0</td><td>-5.74391</td><td>-1.26968</td><td>-0.4008</td></tr> <tr><td>Br</td><td>0</td><td>2.20209</td><td>-3.01175</td><td>0.41739</td></tr> <tr><td>O</td><td>0</td><td>-3.83639</td><td>-0.81928</td><td>-2.72102</td></tr> <tr><td>H</td><td>0</td><td>-4.11482</td><td>0.00618</td><td>1.70732</td></tr> <tr><td>H</td><td>0</td><td>-1.4739</td><td>0.42837</td><td>-2.44961</td></tr> <tr><td>H</td><td>0</td><td>4.1406</td><td>1.53787</td><td>-0.6094</td></tr> <tr><td>H</td><td>0</td><td>0.03008</td><td>-1.0995</td><td>0.13379</td></tr> <tr><td>H</td><td>0</td><td>-3.23514</td><td>-0.67635</td><td>-3.46003</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -13481.5906048 Hartree</td></tr> </table>	O	0	-0.35729	1.51418	-0.38101	C	0	0.83241	0.8401	-0.31178	C	0	2.00349	1.58031	-0.518	C	0	3.24172	0.95926	-0.44787	C	0	3.33775	-0.4059	-0.17397	C	0	2.17254	-1.14516	0.0321	C	0	0.92746	-0.52087	-0.03619	Br	0	5.07822	-1.18056	-0.10126	Br	0	1.90612	3.44297	-0.90118	Br	0	-1.61969	1.4227	2.46257	Br	0	-5.74391	-1.26968	-0.4008	Br	0	2.20209	-3.01175	0.41739	O	0	-3.83639	-0.81928	-2.72102	H	0	-4.11482	0.00618	1.70732	H	0	-1.4739	0.42837	-2.44961	H	0	4.1406	1.53787	-0.6094	H	0	0.03008	-1.0995	0.13379	H	0	-3.23514	-0.67635	-3.46003	<i>E</i> = -13481.5906048 Hartree					<table style="width: 100%; border-collapse: collapse;"> <tr><td>O</td><td>0</td><td>0.13218</td><td>-1.39847</td><td>0.93458</td></tr> <tr><td>C</td><td>0</td><td>1.31326</td><td>-0.70004</td><td>0.91734</td></tr> <tr><td>C</td><td>0</td><td>2.26736</td><td>-0.94426</td><td>-0.07336</td></tr> <tr><td>C</td><td>0</td><td>3.52194</td><td>-0.30861</td><td>-0.03811</td></tr> <tr><td>C</td><td>0</td><td>3.78597</td><td>0.57673</td><td>1.0126</td></tr> <tr><td>C</td><td>0</td><td>2.83908</td><td>0.81936</td><td>2.00416</td></tr> <tr><td>C</td><td>0</td><td>1.60539</td><td>0.18131</td><td>1.96756</td></tr> <tr><td>Br</td><td>0</td><td>5.44596</td><td>1.50363</td><td>1.16855</td></tr> <tr><td>Br</td><td>0</td><td>1.79983</td><td>-2.16735</td><td>-1.44963</td></tr> <tr><td>Br</td><td>0</td><td>-5.23537</td><td>1.06761</td><td>-0.50488</td></tr> <tr><td>Br</td><td>0</td><td>-2.34907</td><td>2.71748</td><td>-1.19064</td></tr> <tr><td>Br</td><td>0</td><td>4.8207</td><td>-0.64454</td><td>-1.38379</td></tr> <tr><td>Br</td><td>0</td><td>-4.98552</td><td>-1.96728</td><td>0.99783</td></tr> <tr><td>O</td><td>0</td><td>0.64203</td><td>0.36035</td><td>2.90737</td></tr> <tr><td>H</td><td>0</td><td>-2.13931</td><td>-2.44521</td><td>1.37144</td></tr> <tr><td>H</td><td>0</td><td>-0.20852</td><td>1.01574</td><td>-0.26128</td></tr> <tr><td>H</td><td>0</td><td>3.07306</td><td>1.50264</td><td>2.81153</td></tr> <tr><td>H</td><td>0</td><td>0.93771</td><td>0.99024</td><td>3.5738</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -16055.1175934 Hartree</td></tr> </table>	O	0	0.13218	-1.39847	0.93458	C	0	1.31326	-0.70004	0.91734	C	0	2.26736	-0.94426	-0.07336	C	0	3.52194	-0.30861	-0.03811	C	0	3.78597	0.57673	1.0126	C	0	2.83908	0.81936	2.00416	C	0	1.60539	0.18131	1.96756	Br	0	5.44596	1.50363	1.16855	Br	0	1.79983	-2.16735	-1.44963	Br	0	-5.23537	1.06761	-0.50488	Br	0	-2.34907	2.71748	-1.19064	Br	0	4.8207	-0.64454	-1.38379	Br	0	-4.98552	-1.96728	0.99783	O	0	0.64203	0.36035	2.90737	H	0	-2.13931	-2.44521	1.37144	H	0	-0.20852	1.01574	-0.26128	H	0	3.07306	1.50264	2.81153	H	0	0.93771	0.99024	3.5738	<i>E</i> = -16055.1175934 Hartree																																																																										
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Br	0	-1.61969	1.4227	2.46257																																																																																																																																																																																																																																																																	
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Br	0	2.20209	-3.01175	0.41739																																																																																																																																																																																																																																																																	
O	0	-3.83639	-0.81928	-2.72102																																																																																																																																																																																																																																																																	
H	0	-4.11482	0.00618	1.70732																																																																																																																																																																																																																																																																	
H	0	-1.4739	0.42837	-2.44961																																																																																																																																																																																																																																																																	
H	0	4.1406	1.53787	-0.6094																																																																																																																																																																																																																																																																	
H	0	0.03008	-1.0995	0.13379																																																																																																																																																																																																																																																																	
H	0	-3.23514	-0.67635	-3.46003																																																																																																																																																																																																																																																																	
<i>E</i> = -13481.5906048 Hartree																																																																																																																																																																																																																																																																					
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C	0	1.31326	-0.70004	0.91734																																																																																																																																																																																																																																																																	
C	0	2.26736	-0.94426	-0.07336																																																																																																																																																																																																																																																																	
C	0	3.52194	-0.30861	-0.03811																																																																																																																																																																																																																																																																	
C	0	3.78597	0.57673	1.0126																																																																																																																																																																																																																																																																	
C	0	2.83908	0.81936	2.00416																																																																																																																																																																																																																																																																	
C	0	1.60539	0.18131	1.96756																																																																																																																																																																																																																																																																	
Br	0	5.44596	1.50363	1.16855																																																																																																																																																																																																																																																																	
Br	0	1.79983	-2.16735	-1.44963																																																																																																																																																																																																																																																																	
Br	0	-5.23537	1.06761	-0.50488																																																																																																																																																																																																																																																																	
Br	0	-2.34907	2.71748	-1.19064																																																																																																																																																																																																																																																																	
Br	0	4.8207	-0.64454	-1.38379																																																																																																																																																																																																																																																																	
Br	0	-4.98552	-1.96728	0.99783																																																																																																																																																																																																																																																																	
O	0	0.64203	0.36035	2.90737																																																																																																																																																																																																																																																																	
H	0	-2.13931	-2.44521	1.37144																																																																																																																																																																																																																																																																	
H	0	-0.20852	1.01574	-0.26128																																																																																																																																																																																																																																																																	
H	0	3.07306	1.50264	2.81153																																																																																																																																																																																																																																																																	
H	0	0.93771	0.99024	3.5738																																																																																																																																																																																																																																																																	
<i>E</i> = -16055.1175934 Hartree																																																																																																																																																																																																																																																																					
<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">6-OH-BDE-140</td></tr> <tr><td>C</td><td>0</td><td>-0.68555</td><td>-0.41296</td><td>1.47743</td></tr> <tr><td>C</td><td>0</td><td>-0.63751</td><td>0.35281</td><td>0.3047</td></tr> <tr><td>C</td><td>0</td><td>-1.81732</td><td>0.60026</td><td>-0.40497</td></tr> <tr><td>C</td><td>0</td><td>-3.0447</td><td>0.06419</td><td>0.0209</td></tr> <tr><td>C</td><td>0</td><td>-3.06167</td><td>-0.72518</td><td>1.17471</td></tr> <tr><td>C</td><td>0</td><td>-1.89337</td><td>-0.95787</td><td>1.89247</td></tr> <tr><td>O</td><td>0</td><td>0.50922</td><td>0.97589</td><td>-0.12369</td></tr> <tr><td>C</td><td>0</td><td>1.75157</td><td>0.39708</td><td>-0.07187</td></tr> <tr><td>C</td><td>0</td><td>2.08729</td><td>-0.7891</td><td>-0.73388</td></tr> <tr><td>C</td><td>0</td><td>3.38793</td><td>-1.28642</td><td>-0.70924</td></tr> <tr><td>C</td><td>0</td><td>4.37019</td><td>-0.57179</td><td>-0.0366</td></tr> <tr><td>C</td><td>0</td><td>4.08103</td><td>0.62796</td><td>0.60327</td></tr> <tr><td>C</td><td>0</td><td>2.77408</td><td>1.09924</td><td>0.57968</td></tr> <tr><td>Br</td><td>0</td><td>2.3725</td><td>2.73568</td><td>1.46805</td></tr> <tr><td>Br</td><td>0</td><td>6.1604</td><td>-1.2446</td><td>-0.00267</td></tr> <tr><td>Br</td><td>0</td><td>0.78322</td><td>-1.76167</td><td>-1.73269</td></tr> <tr><td>Br</td><td>0</td><td>-4.65992</td><td>-1.52149</td><td>1.84833</td></tr> <tr><td>Br</td><td>0</td><td>-4.64247</td><td>0.39964</td><td>-0.95242</td></tr> <tr><td>Br</td><td>0</td><td>-1.68841</td><td>1.68426</td><td>-1.9592</td></tr> <tr><td>O</td><td>0</td><td>0.47541</td><td>-0.58709</td><td>2.16833</td></tr> <tr><td>H</td><td>0</td><td>-1.92967</td><td>-1.55941</td><td>2.79284</td></tr> <tr><td>H</td><td>0</td><td>3.62395</td><td>-2.2076</td><td>-1.22247</td></tr> <tr><td>H</td><td>0</td><td>4.85068</td><td>1.18577</td><td>1.11702</td></tr> <tr><td>H</td><td>0</td><td>0.31991</td><td>-1.1322</td><td>2.94712</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -16055.1162060 Hartree</td></tr> </table>	6-OH-BDE-140					C	0	-0.68555	-0.41296	1.47743	C	0	-0.63751	0.35281	0.3047	C	0	-1.81732	0.60026	-0.40497	C	0	-3.0447	0.06419	0.0209	C	0	-3.06167	-0.72518	1.17471	C	0	-1.89337	-0.95787	1.89247	O	0	0.50922	0.97589	-0.12369	C	0	1.75157	0.39708	-0.07187	C	0	2.08729	-0.7891	-0.73388	C	0	3.38793	-1.28642	-0.70924	C	0	4.37019	-0.57179	-0.0366	C	0	4.08103	0.62796	0.60327	C	0	2.77408	1.09924	0.57968	Br	0	2.3725	2.73568	1.46805	Br	0	6.1604	-1.2446	-0.00267	Br	0	0.78322	-1.76167	-1.73269	Br	0	-4.65992	-1.52149	1.84833	Br	0	-4.64247	0.39964	-0.95242	Br	0	-1.68841	1.68426	-1.9592	O	0	0.47541	-0.58709	2.16833	H	0	-1.92967	-1.55941	2.79284	H	0	3.62395	-2.2076	-1.22247	H	0	4.85068	1.18577	1.11702	H	0	0.31991	-1.1322	2.94712	<i>E</i> = -16055.1162060 Hartree					<table style="width: 100%; border-collapse: collapse;"> <tr><td colspan="5" style="text-align: center;">3'-OH-BDE-154</td></tr> <tr><td>C</td><td>0</td><td>3.36388</td><td>0.95228</td><td>-0.07125</td></tr> <tr><td>C</td><td>0</td><td>2.11668</td><td>1.55913</td><td>-0.04706</td></tr> <tr><td>C</td><td>0</td><td>0.95864</td><td>0.77641</td><td>0.01849</td></tr> <tr><td>C</td><td>0</td><td>1.07071</td><td>-0.60863</td><td>0.05936</td></tr> <tr><td>C</td><td>0</td><td>2.32446</td><td>-1.21816</td><td>0.03532</td></tr> <tr><td>C</td><td>0</td><td>3.47905</td><td>-0.43783</td><td>-0.03051</td></tr> <tr><td>O</td><td>0</td><td>-0.24445</td><td>1.43695</td><td>0.04152</td></tr> <tr><td>C</td><td>0</td><td>-1.42295</td><td>0.73797</td><td>0.09397</td></tr> <tr><td>C</td><td>0</td><td>-2.08269</td><td>0.39534</td><td>-1.0912</td></tr> <tr><td>C</td><td>0</td><td>-3.33577</td><td>-0.23595</td><td>-1.06072</td></tr> <tr><td>C</td><td>0</td><td>-3.9013</td><td>-0.50526</td><td>0.19261</td></tr> <tr><td>C</td><td>0</td><td>-3.26442</td><td>-0.16349</td><td>1.37663</td></tr> <tr><td>C</td><td>0</td><td>-2.02434</td><td>0.46156</td><td>1.3265</td></tr> <tr><td>Br</td><td>0</td><td>-5.61347</td><td>-1.36517</td><td>0.25094</td></tr> <tr><td>Br</td><td>0</td><td>-1.2946</td><td>0.79618</td><td>-2.76909</td></tr> <tr><td>Br</td><td>0</td><td>5.23111</td><td>-1.18873</td><td>-0.06874</td></tr> <tr><td>Br</td><td>0</td><td>2.38027</td><td>-3.12239</td><td>0.09576</td></tr> <tr><td>O</td><td>0</td><td>-3.93231</td><td>-0.54648</td><td>-2.22695</td></tr> <tr><td>Br</td><td>0</td><td>-1.15879</td><td>0.95409</td><td>2.95003</td></tr> <tr><td>Br</td><td>0</td><td>1.99271</td><td>3.45735</td><td>-0.10456</td></tr> <tr><td>H</td><td>0</td><td>4.25478</td><td>1.56263</td><td>-0.12248</td></tr> <tr><td>H</td><td>0</td><td>0.18103</td><td>-1.22111</td><td>0.10995</td></tr> <tr><td>H</td><td>0</td><td>-3.72927</td><td>-0.37672</td><td>2.3287</td></tr> <tr><td>H</td><td>0</td><td>-4.78712</td><td>-0.96574</td><td>-2.04742</td></tr> <tr><td colspan="5" style="text-align: center;"><i>E</i> = -16055.1288874 Hartree</td></tr> </table>	3'-OH-BDE-154					C	0	3.36388	0.95228	-0.07125	C	0	2.11668	1.55913	-0.04706	C	0	0.95864	0.77641	0.01849	C	0	1.07071	-0.60863	0.05936	C	0	2.32446	-1.21816	0.03532	C	0	3.47905	-0.43783	-0.03051	O	0	-0.24445	1.43695	0.04152	C	0	-1.42295	0.73797	0.09397	C	0	-2.08269	0.39534	-1.0912	C	0	-3.33577	-0.23595	-1.06072	C	0	-3.9013	-0.50526	0.19261	C	0	-3.26442	-0.16349	1.37663	C	0	-2.02434	0.46156	1.3265	Br	0	-5.61347	-1.36517	0.25094	Br	0	-1.2946	0.79618	-2.76909	Br	0	5.23111	-1.18873	-0.06874	Br	0	2.38027	-3.12239	0.09576	O	0	-3.93231	-0.54648	-2.22695	Br	0	-1.15879	0.95409	2.95003	Br	0	1.99271	3.45735	-0.10456	H	0	4.25478	1.56263	-0.12248	H	0	0.18103	-1.22111	0.10995	H	0	-3.72927	-0.37672	2.3287	H	0	-4.78712	-0.96574	-2.04742	<i>E</i> = -16055.1288874 Hartree				
6-OH-BDE-140																																																																																																																																																																																																																																																																					
C	0	-0.68555	-0.41296	1.47743																																																																																																																																																																																																																																																																	
C	0	-0.63751	0.35281	0.3047																																																																																																																																																																																																																																																																	
C	0	-1.81732	0.60026	-0.40497																																																																																																																																																																																																																																																																	
C	0	-3.0447	0.06419	0.0209																																																																																																																																																																																																																																																																	
C	0	-3.06167	-0.72518	1.17471																																																																																																																																																																																																																																																																	
C	0	-1.89337	-0.95787	1.89247																																																																																																																																																																																																																																																																	
O	0	0.50922	0.97589	-0.12369																																																																																																																																																																																																																																																																	
C	0	1.75157	0.39708	-0.07187																																																																																																																																																																																																																																																																	
C	0	2.08729	-0.7891	-0.73388																																																																																																																																																																																																																																																																	
C	0	3.38793	-1.28642	-0.70924																																																																																																																																																																																																																																																																	
C	0	4.37019	-0.57179	-0.0366																																																																																																																																																																																																																																																																	
C	0	4.08103	0.62796	0.60327																																																																																																																																																																																																																																																																	
C	0	2.77408	1.09924	0.57968																																																																																																																																																																																																																																																																	
Br	0	2.3725	2.73568	1.46805																																																																																																																																																																																																																																																																	
Br	0	6.1604	-1.2446	-0.00267																																																																																																																																																																																																																																																																	
Br	0	0.78322	-1.76167	-1.73269																																																																																																																																																																																																																																																																	
Br	0	-4.65992	-1.52149	1.84833																																																																																																																																																																																																																																																																	
Br	0	-4.64247	0.39964	-0.95242																																																																																																																																																																																																																																																																	
Br	0	-1.68841	1.68426	-1.9592																																																																																																																																																																																																																																																																	
O	0	0.47541	-0.58709	2.16833																																																																																																																																																																																																																																																																	
H	0	-1.92967	-1.55941	2.79284																																																																																																																																																																																																																																																																	
H	0	3.62395	-2.2076	-1.22247																																																																																																																																																																																																																																																																	
H	0	4.85068	1.18577	1.11702																																																																																																																																																																																																																																																																	
H	0	0.31991	-1.1322	2.94712																																																																																																																																																																																																																																																																	
<i>E</i> = -16055.1162060 Hartree																																																																																																																																																																																																																																																																					
3'-OH-BDE-154																																																																																																																																																																																																																																																																					
C	0	3.36388	0.95228	-0.07125																																																																																																																																																																																																																																																																	
C	0	2.11668	1.55913	-0.04706																																																																																																																																																																																																																																																																	
C	0	0.95864	0.77641	0.01849																																																																																																																																																																																																																																																																	
C	0	1.07071	-0.60863	0.05936																																																																																																																																																																																																																																																																	
C	0	2.32446	-1.21816	0.03532																																																																																																																																																																																																																																																																	
C	0	3.47905	-0.43783	-0.03051																																																																																																																																																																																																																																																																	
O	0	-0.24445	1.43695	0.04152																																																																																																																																																																																																																																																																	
C	0	-1.42295	0.73797	0.09397																																																																																																																																																																																																																																																																	
C	0	-2.08269	0.39534	-1.0912																																																																																																																																																																																																																																																																	
C	0	-3.33577	-0.23595	-1.06072																																																																																																																																																																																																																																																																	
C	0	-3.9013	-0.50526	0.19261																																																																																																																																																																																																																																																																	
C	0	-3.26442	-0.16349	1.37663																																																																																																																																																																																																																																																																	
C	0	-2.02434	0.46156	1.3265																																																																																																																																																																																																																																																																	
Br	0	-5.61347	-1.36517	0.25094																																																																																																																																																																																																																																																																	
Br	0	-1.2946	0.79618	-2.76909																																																																																																																																																																																																																																																																	
Br	0	5.23111	-1.18873	-0.06874																																																																																																																																																																																																																																																																	
Br	0	2.38027	-3.12239	0.09576																																																																																																																																																																																																																																																																	
O	0	-3.93231	-0.54648	-2.22695																																																																																																																																																																																																																																																																	
Br	0	-1.15879	0.95409	2.95003																																																																																																																																																																																																																																																																	
Br	0	1.99271	3.45735	-0.10456																																																																																																																																																																																																																																																																	
H	0	4.25478	1.56263	-0.12248																																																																																																																																																																																																																																																																	
H	0	0.18103	-1.22111	0.10995																																																																																																																																																																																																																																																																	
H	0	-3.72927	-0.37672	2.3287																																																																																																																																																																																																																																																																	
H	0	-4.78712	-0.96574	-2.04742																																																																																																																																																																																																																																																																	
<i>E</i> = -16055.1288874 Hartree																																																																																																																																																																																																																																																																					